1,2-Naphthalenedione, 3,8-dimethyl-5-(1-methylethyl)-5574-34-5 | DTXSID80204286

| 3374-34-3 DTA3ID00204200 | | | | | | |
|----------------------------|--|--|--|--|--|--|
| | | | | | | |
| | | | | | | |
| | | | | | | |

Model Performance

| Model | Data |
|---------|------|
| IVIOGCI | Data |

Weighted KNN model

| 5-fold CV | 5-fold CV (75%) Training (75%) | | 5-fold CV (75%) | | Test (25% | ·) | |
|-----------|--------------------------------|------|-----------------|------|-----------|----|--|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE | | |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 | | |

Model Results

Predicted value: 6.23e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.48e-01

Confidence level: 4.74e-01

Nearest Neighbors from the Training Set

Image not found

Isouron

Measured: 1.20e-06 Predicted: 1.37e-06

Image not found

Fluridone

Measured: 3.30e-06 Predicted: 8.69e-08

Image not found

C.I. Disperse Blue 1 Measured: 8.45e-08 Predicted: 1.43e-08

Image not found

Furathiocarb

Measured: 2.78e-06 Predicted: 5.50e-08

Image not found

4-Aminoazobenzene Measured: 7.00e-08 Predicted: 1.49e-06